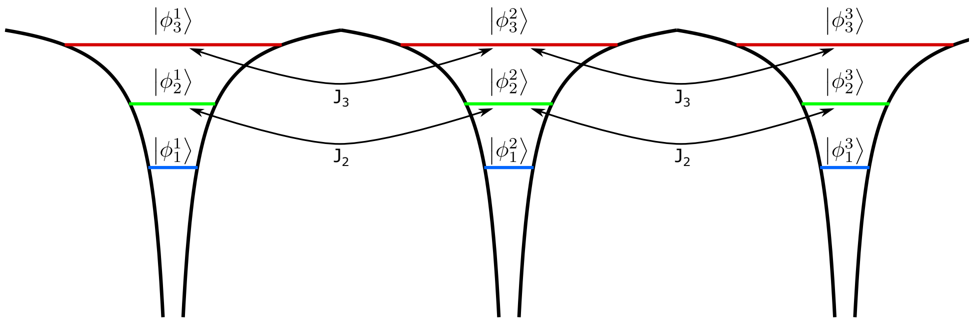
Tutorial 4 - Tight binding model

Let us consider N atoms regularly spaced with a distance a - which is a generalization of the double well situation discussed in the first chapter. We will note $h_0^{(n)}$ the Hamiltonian corresponding to the n^{th} atom alone. The eigenstates of $h_0^{(n)}$ are noted $\left|\phi_j^{(n)}\right\rangle$ with energies E_k. Because of the tunnel effect, an electron can jump from one atom to the next one. We note J_j the coupling strength between the j^{th} energy state of two neighboring atoms - and we assume that the electron can only jump to its nearest neighbor, and cannot jump from from one energy state to another.



Reminder

- In the presence of a trapping potential, the Hamiltonian eigenstates take discrete energy values, and can be labeled by an integer number n.
- Any coupling between states tends to lift degeneracies. The eigenstates are then delocalized. The resulting energy splitting is larger if the coupling is stronger.

Like in chapter 1, we consider $H = H_0 + V$ with

$$H_0 \left|\phi_j^n\right\rangle = E_j \left|\phi_j^n\right\rangle \tag{1}$$

$$V \left|\phi_j^n\right\rangle = -J_j \left(\left|\phi_j^{n-1}\right\rangle + \left|\phi_j^{n+1}\right\rangle\right) \tag{2}$$

and we will look for the eigenstates $\left\{\left|\psi_j\right\rangle\right\}$ of this total Hamiltonian resulting from the E_j manifold (ie from all states sharing the same energy E_j in absence of coupling).

Part 1: calculating the band diagram

1. Justify that we can write $\left|\psi_j\right\rangle$ as $\left|\psi_j\right\rangle = \sum\limits_n c_j^n \left|\phi_j^n\right\rangle$.
2. Show that the $\left\{c_j^n\right\}$ coefficients follow the relation

$$E\, c_j^n = E_j\, c_j^n - J_j\, \left(c_j^{n-1} + c_j^{n+1}\right) \tag{3}$$

   where E is the energy of the eigenstate $\left|\psi_j\right\rangle$.
3. It can be shown that eigenfunctions of H have to obey

$$\psi_j(x+a) = e^{ika}\psi_j(x) \tag{4}$$

   with $k = 2p\pi/Na$, $p \in \mathbb{Z}$ (Bloch theorem). Assuming this result, show that the $\left\{c_j^n\right\}$ coefficients follow the relation

$$c_j^n = c_j^0\, \exp\left(i\, n\, k\, a\right) \tag{5}$$

Hint: use the fact that each of the $\left\{\phi_j^n\right\}_{j\in[1,N]}$ *functions is the same function* $\phi^n(x)$ *simply shifted by a distance* $j \times a$ *to be centered around the* j^{th} *atom.*

4. Find the dispersion relation of this system and draw it. Show that all the information about the dispersion relation is contained in the interval $k \in [-\pi/a, \pi/a]$. Identify energy bands, and energy gaps.

Part 2: properties of electrons in this system

5. Consider that, in the absence of coupling, each atom is occupied by 3 electrons. We now turn on the coupling between atoms, leading to the aforementioned energy bands. How are these bands populated at $T = 0$ K? Where does the Fermi level lies?
   (a) What happens if we try to bring the system out of thermal equilibrium by adding a tiny bit of energy to it (for instance, adding an electron field to drive electrons)?
6. Consider that, in the absence of coupling, each atom is occupied by 4 electrons. We now turn on the coupling between atoms, leading to the aforementioned energy bands. How are these bands populated at $T = 0$ K? Identify the valence and conduction band. Where does the Fermi level lies?
   (b) What happens if we try to bring the system out of thermal equilibrium by adding a tiny bit of energy to it (for instance, adding an electron field to drive electrons)?
   (c) Show that, close to the bottom or to the top of a band, the dispersion relation looks like that of free particles. Express the density of states sligthly above and slightly below the Fermi level.
   (d) At temperature $T > 0$K, some electrons can be found above the Fermi level, leaving some empty state below the Fermi level. Considering that the Fermi level is far from both the edges of both the conduction and the valence bands, estimate the density n of electrons present in the conduction band and the density p of electrons *missing* in the valence band.
   (e) Using charge neutrality, evaluate the exacte position of the Fermi level.
   (f) Considering that only electrons in the conduction band are able to contribute to a net electrical current, show that, at room temperature, the material is an insulator if its energy gap is larger than few electron-volts.